Grains

R. Hielscher

Faculty of Mathematics,
Chemnitz University of Technology, Germany

2019

Setting up an EBSD map

1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising

Setting up an EBSD map

1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising

Setting up an EBSD map

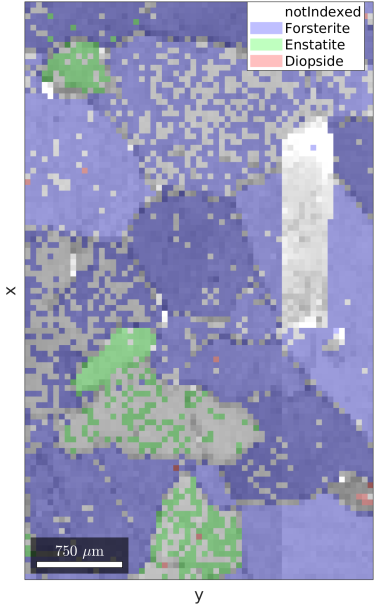
1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising

Setting up an EBSD map

1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising

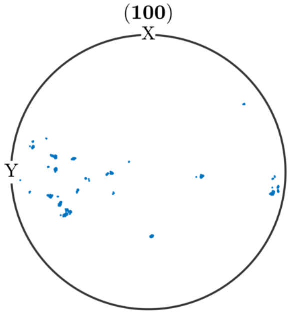
Setting up an EBSD map

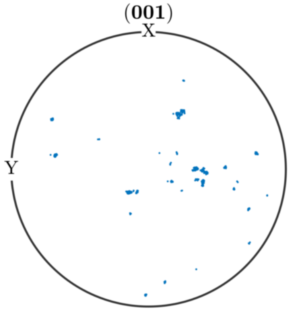
1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising



Setting up an EBSD map

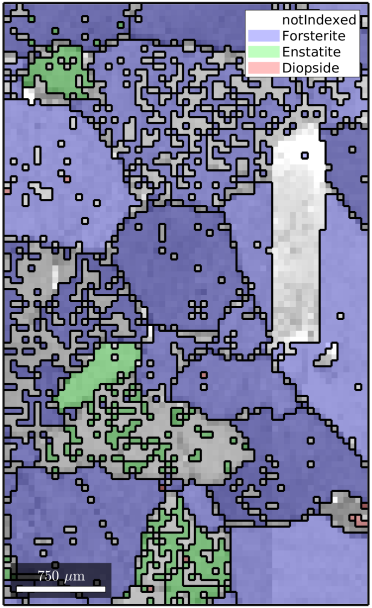
1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising





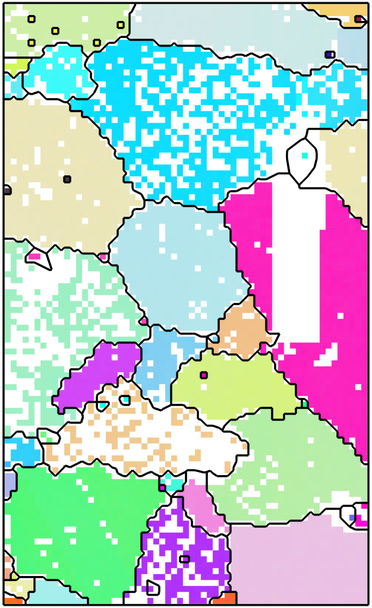
Setting up an EBSD map

1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising



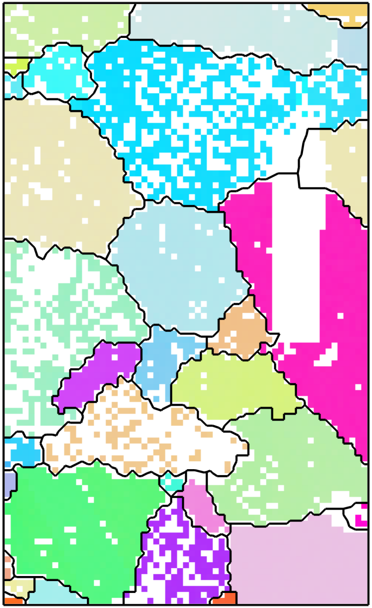
Setting up an EBSD map

1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising



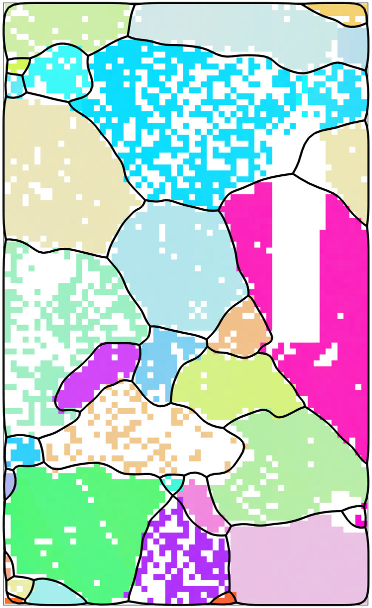
Setting up an EBSD map

1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising



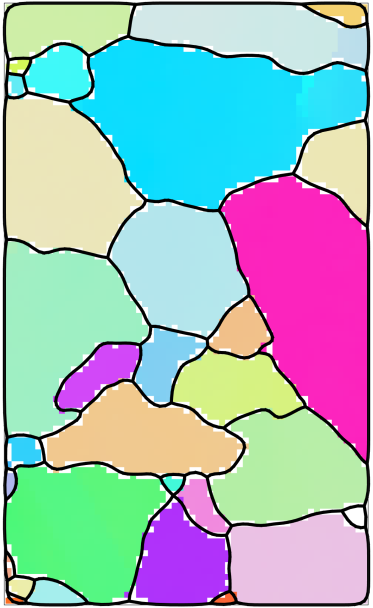
Setting up an EBSD map

1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising



Setting up an EBSD map

1. ensure all correct symmetry groups for all phases
2. ensure all correct lattice parameters a, b, c, α, β, γ
3. ensure correct alignment of the symmetry axes
4. ensure correct alignment of $\vec{a}$, $\vec{b}$, $\vec{c}$
5. align the EBSD map with respect to the specimen
6. align the pole figures with respect to the specimen
7. reconstruct a grain structure
8. remove purely indexed measurements,
   e.g. one pixel grains, low band constrast
9. reconstruction grain structure
10. grain boundary smoothing
11. orientation denoising



What are Grains?

Definition

A grain or a crystallite is a small or even microscopic crystal which forms, for example, during the cooling of many materials.

The areas where crystallites meet are called grain boundaries.

Shape, alignment and size of the grains have a big impact on macroscopic properties.

The above grain definition is not sufficiently exact.

Definition

A plane is called a grain boundary if the orientation of the crystal lattices on both sides differ by more then a certain threshold.

Grain are connected regions enclosed by grain boundaries.

What are Grains?

Definition

A grain or a crystallite is a small or even microscopic crystal which forms, for example, during the cooling of many materials.

The areas where crystallites meet are called grain boundaries.

Shape, alignment and size of the grains have a big impact on macroscopic properties.

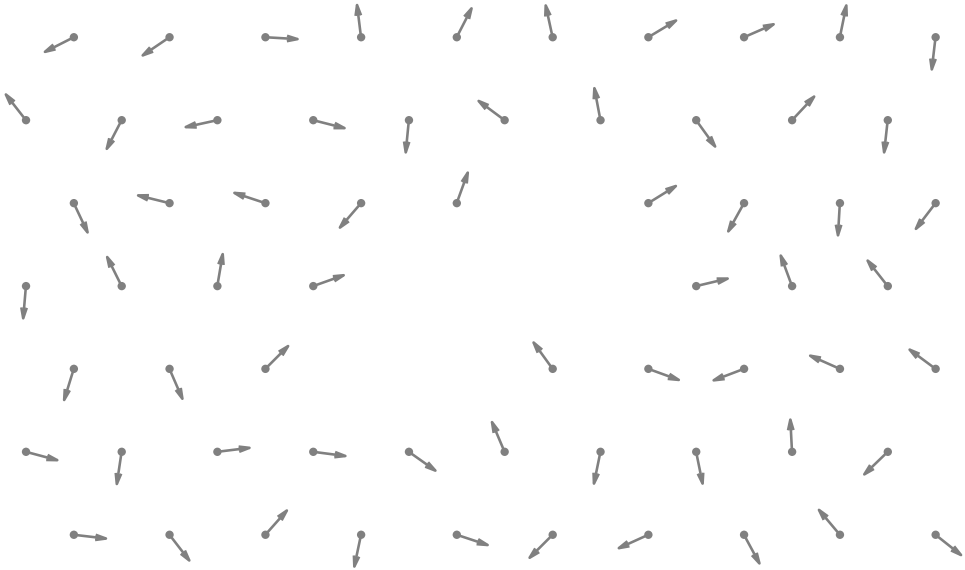
The above grain definition is not sufficiently exact.

Definition

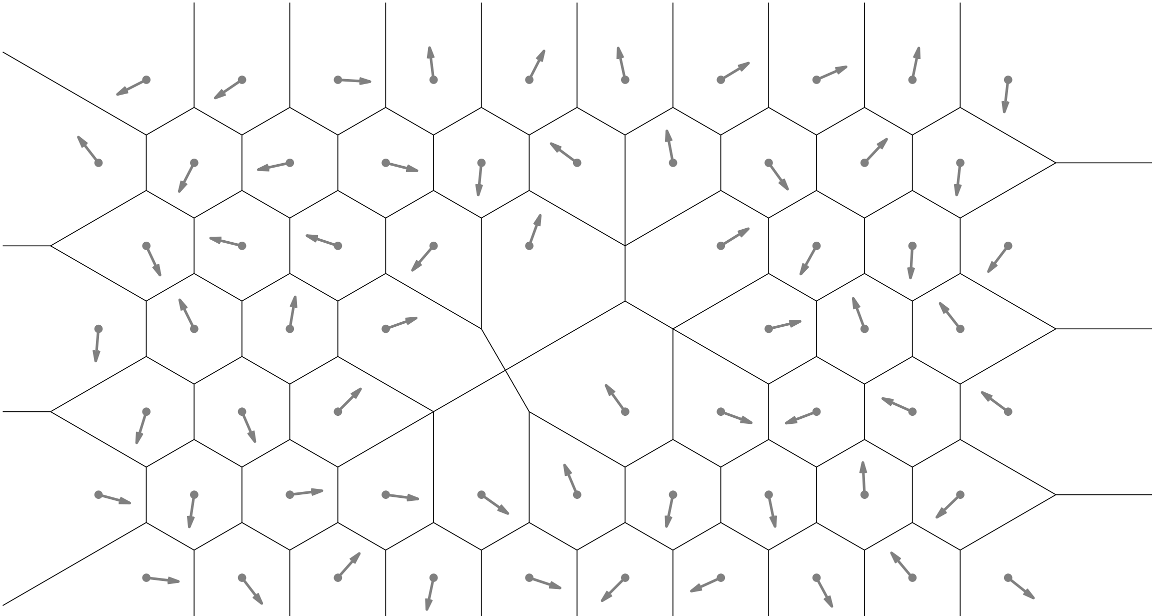
A plane is called a grain boundary if the orientation of the crystal lattices on both sides differ by more then a certain threshold.

Grain are connected regions enclosed by grain boundaries.

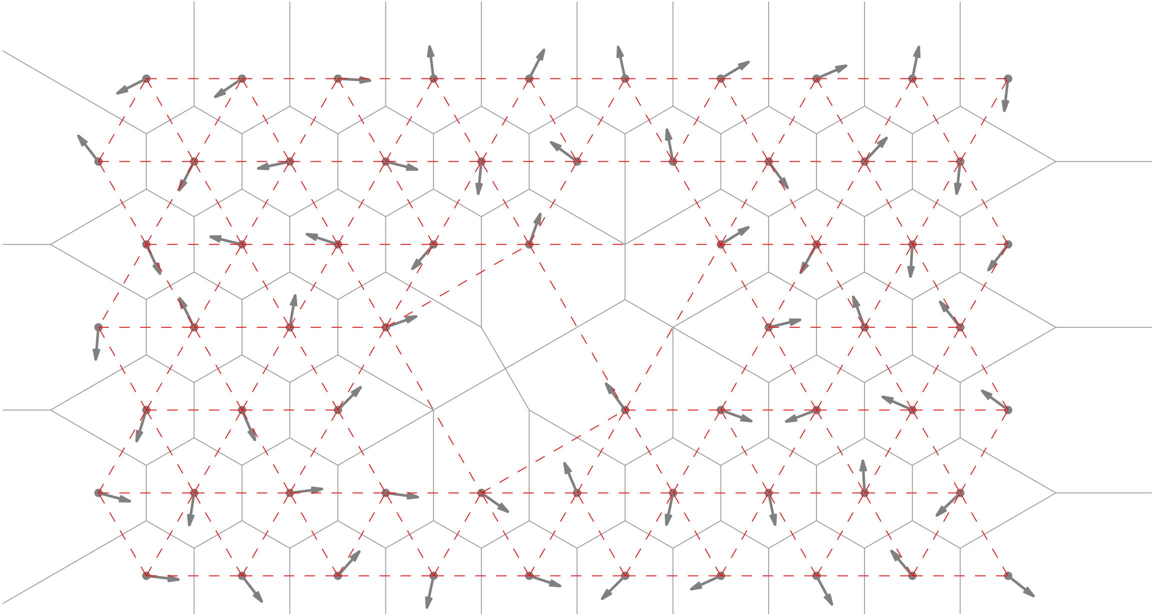
A Threshold Based Segmentation Algorithm



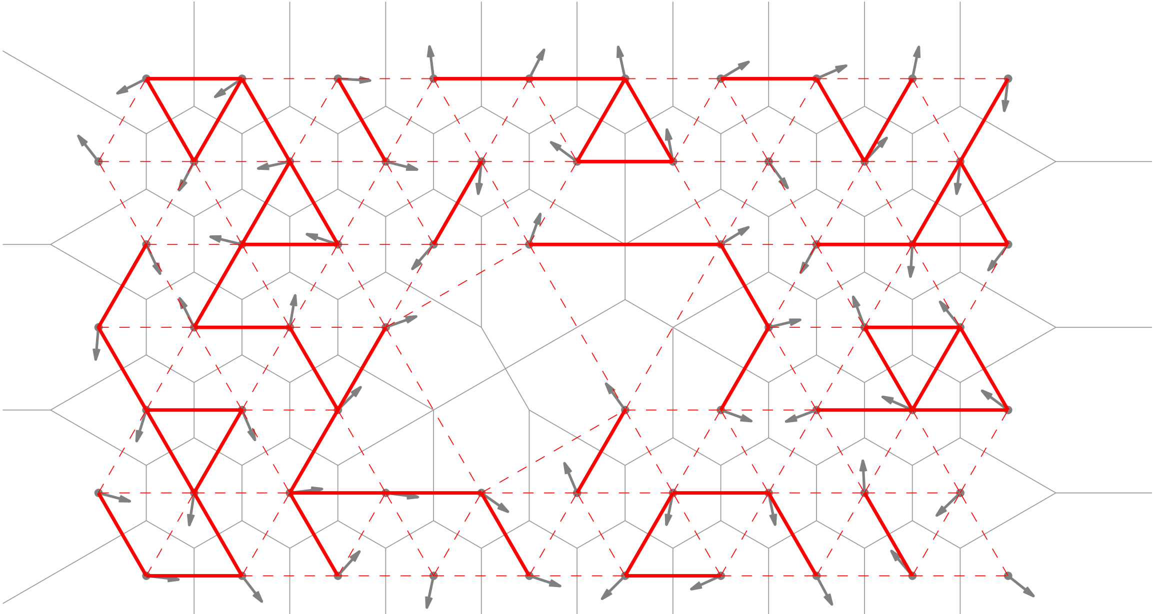
A Threshold Based Segmentation Algorithm



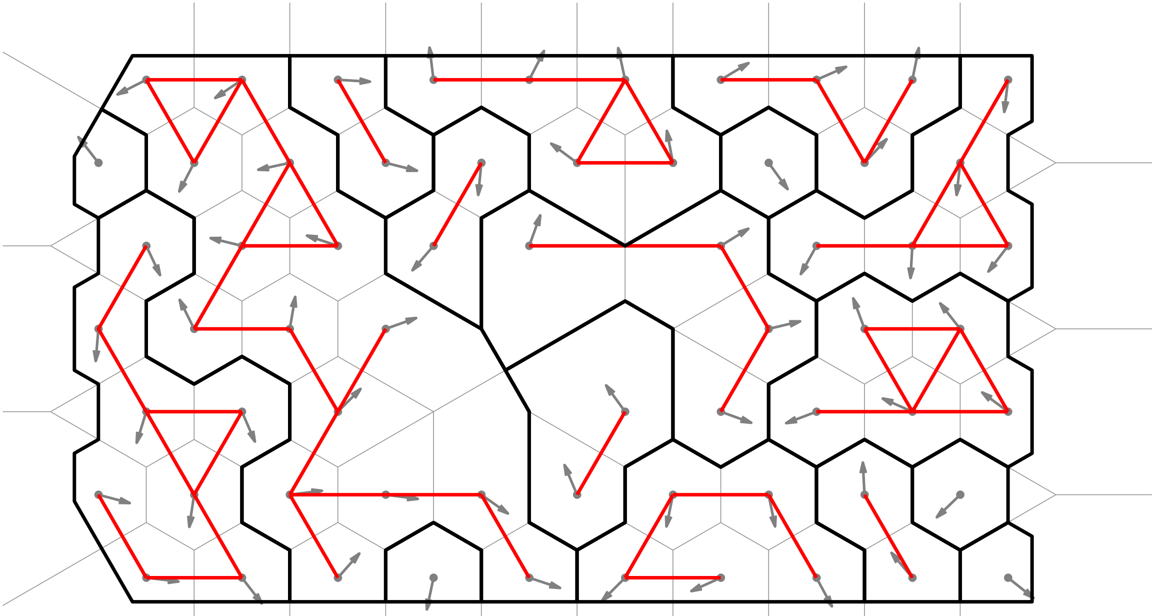
A Threshold Based Segmentation Algorithm



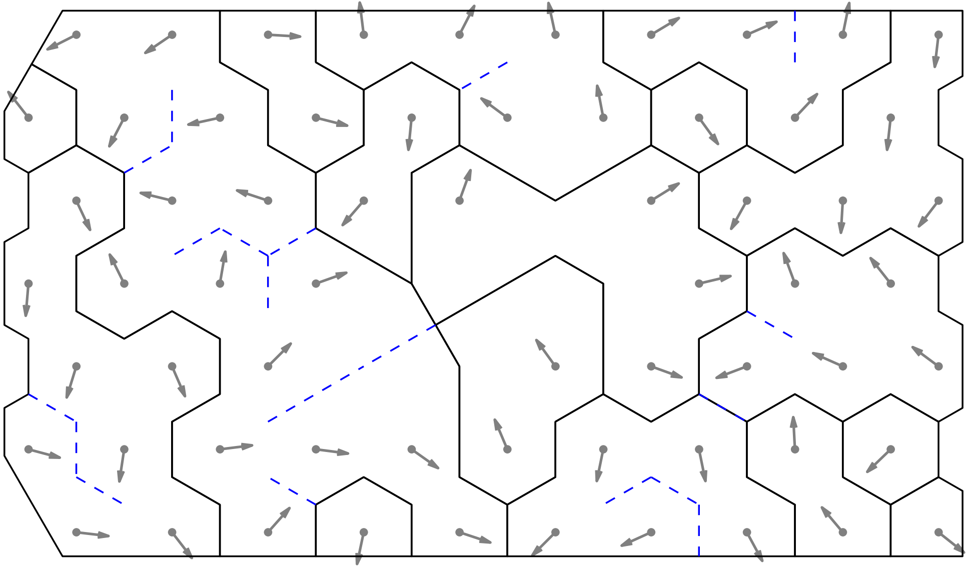
A Threshold Based Segmentation Algorithm



A Threshold Based Segmentation Algorithm



A Threshold Based Segmentation Algorithm



Properties of the Segmentation Algorithm

- not indexed pixels can be considered as no information and their area is distributed between adjacent measurements
- one can consider a big not indexed area as a “not indexed” phase to prevent it to be distributed
- typical rectangular or hexagonal grids lead to a stair casing effects at grain boundaries
- this effect is reduced if measurement along the grain boundaries are classified as not indexed
- grains may be connected by a single pixel

MTEX

```
% reconstruct grains with a specific threshold angle
[grains,ebsd.grainId,ebsd.mis2mean] = ...
          calcGrains(ebsdP('indexed'),'angle',10*degree)

grains = smooth(grains,5) % smooth grains

% grain properties
grains.meanOrientation
grains.id           % -> ebsd.grainId
grains.V            % the vertices of all grains
grains.x, grains.x
grains.poly         % indices to V that form the grain
grains.centroid     % midpoint
grains.grainSize    % number of measurements per grain
grains.area         % area per grain
grains.size         % number of grains
```

MTEX

```
grains.neighbours % number of neighbors
grains.hasHole

grains.boundary      % list of outer boundary segments
grains.innerBoundary % list of inner boundary segments
grains.boundarySize % number of segments per grain

grains.GOS           % grain orientation spread
```

Grain Boundaries

```
gB = grains.boundary

gB.grainId
gB.ebsdId
gB.phaseId
gB.segLength
gB.midPoint
gB.misorientation

gB.componentId
gB.componentSize
```

Geometrical Grain Properties

Grain shape parameters:

- area
- diameter
- perimeter
- paris
- fitted ellipse
- aspect ratio
- shape factor

Texture Related Grain Properties

Mean Orientation:

$$\overline{\mathbf{O}}_G = \underset{\mathbf{O}}{\operatorname{argmin}} \sum_{(i,j)\in G} \omega(\mathbf{O}_{i,j}, \mathbf{O})^2$$

Grain Orientation Spread (GOS):

$$\mathrm{GOS} = \sum_{(i,j)\in G} \omega(\mathbf{O}_{i,j}, \overline{\mathbf{O}}_G)$$

Grain Average Misorientation (GAM):

$$\mathrm{GAM} = \sum_{(i,j)\in G} \omega(\mathbf{O}_{i,j}, \mathbf{O}_{i,j+1}) + \omega(\mathbf{O}_{i,j}, \mathbf{O}_{i+1,j})$$

GOS and GAM are often used to detect and quantify the deformed or recrystallized grains.

Texture Related Grain Properties

Mean Orientation:

$$\overline{\mathbf{O}}_G = \operatorname*{argmin}_{\mathbf{O}} \sum_{(i,j)\in G} \omega(\mathbf{O}_{i,j}, \mathbf{O})^2$$

Grain Orientation Spread (GOS):

$$\mathrm{GOS} = \sum_{(i,j)\in G} \omega(\mathbf{O}_{i,j}, \overline{\mathbf{O}}_G)$$

Grain Average Misorientation (GAM):

$$\mathrm{GAM} = \sum_{(i,j)\in G} \omega(\mathbf{O}_{i,j}, \mathbf{O}_{i,j+1}) + \omega(\mathbf{O}_{i,j}, \mathbf{O}_{i+1,j})$$

GOS and GAM are often used to detect and quantify the deformed or recrystallized grains.

Texture Related Grain Properties

Mean Orientation:

$$\overline{\mathbf{O}}_G = \operatorname*{argmin}_{\mathbf{O}} \sum_{(i,j)\in G} \omega(\mathbf{O}_{i,j}, \mathbf{O})^2$$

Grain Orientation Spread (GOS):

$$\mathrm{GOS} = \sum_{(i,j)\in G} \omega(\mathbf{O}_{i,j}, \overline{\mathbf{O}}_G)$$

Grain Average Misorientation (GAM):

$$\mathrm{GAM} = \sum_{(i,j)\in G} \omega(\mathbf{O}_{i,j}, \mathbf{O}_{i,j+1}) + \omega(\mathbf{O}_{i,j}, \mathbf{O}_{i+1,j})$$

GOS and GAM are often used to detect and quantify the deformed or recrystallized grains.

Grain Boundary Smoothing

Goals:

1. Find a more realistic staircase free grain boundary.
2. Do not move triple points.

This can be achieved by solving the minimization problem

$$J(\gamma) = \sum_{i=1}^{I} \|\gamma(t_i) x_i\|^2 + \lambda \|\triangle \gamma\|_2^2 \to \min$$

with $\gamma(t_i) = x_i$ for all triple points x_i.

Recursion: $\vec{x}_i^{k+1} = \lambda \vec{x}_i^k + (1+\lambda)\frac{\vec{x}_{i+1}^k + \vec{x}_{i-1}^k}{2}$

Properties: Larger Grains grow on the cost of smaller grains.

Grain Boundary Smoothing

Goals:

1. Find a more realistic staircase free grain boundary.
2. Do not move triple points.

This can be achieved by solving the minimization problem

$$J(\gamma) = \sum_{i=1}^{I} \|\gamma(t_i) x_i\|^2 + \lambda \|\triangle \gamma\|_2^2 \to \min$$

with $\gamma(t_i) = x_i$ for all triple points x_i.

Recursion: $\vec{x}_i^{k+1} = \lambda \vec{x}_i^k + (1+\lambda) \frac{\vec{x}_{i+1}^k + \vec{x}_{i-1}^k}{2}$

Properties: Larger Grains grow on the cost of smaller grains.

Denoising of EBSD Maps

see extra presentation